

# RENORMALIZED PERTURBATION APPROACH TO ELECTRON TRANSPORT THROUGH QUANTUM DOT

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**Abstract.** We review the basic ideas of a renormalized perturbation theory which works directly in terms of fully dressed quasiparticles, and its application to the calculation of the current through a quantum dot both in equilibrium and non-equilibrium steady state conditions. The method is illustrated for the impurity Anderson model. We show how the relevant renormalized parameters can be deduced from a numerical renormalization group calculation, and also how they can be generalized to include an arbitrary magnetic field. In applying the method to electron transmission through quantum dot, we show how the zero field conductance can be expressed in terms of the renormalized parameters, and how asymptotically exact results at low bias voltages can be derived from the expansion to second order. The potential for the further application of this approach to this class of problems is assessed.

**Key words:** electron transport, quantum dot, impurity, electron chain.

## 2.1 Introduction

The problems of the infinities that arose in the early application of perturbation theory to quantum electrodynamics (QED) in the 1940s were eventually circumvented by reorganising the perturbation expansion so that it could be made in terms of the ‘fully dressed’ electrons, rather than the original or ‘bare’ electrons [1]. The renormalized parameters describing the fully dressed electrons, their mass, charge, and the rescaled fields in the low energy regime could then be taken directly from experiment. In the reorganized perturbation theory, counter terms have to be included to prevent overcounting and renormalizing quantities which have already been taken as being fully renormalized.

The theory can then be developed entirely in terms of the renormalized parameters. The success of this approach not only led to elimination of all reference to divergent quantities but, as is well known, gave results for quantities such as the  $g$ -factor for the electron in unprecedentedly precise agreement with experiment. The divergence problems in QED arose from the lack of a high energy cut-off. In the field of condensed matter theory, there is always a relevant finite cut-off, so this approach to renormalization has seldom been used. Strong renormalization effects, however, are a characteristic of strongly correlated electron systems in condensed matter, such as heavy fermions where the effective mass of the electrons at low temperatures can be of the order of 1,000 times that of a ‘bare’ electron. The approaches to renormalization used in condensed matter have, for the most part, been based on the methods developed by Wilson for the calculation of critical exponents, where shorter wavelength or higher energy fluctuations are progressively integrated out to derive an effective theory for the long wavelength or low energy states [2]. The advantage of this approach, when it can be carried out fully, is that the renormalized parameters for the effective model describing the low energy or long wave fluctuations can be calculated explicitly. The complications that arise are that new interaction terms are generated on intermediate scales in the process, which can be very difficult to handle. Here we show some of the merits of combining the Wilson approach with the earlier one of working with a renormalized perturbation theory in terms of fully dressed quasiparticles, particularly for calculating the low energy behavior for strongly correlated electron systems. We show how this combined approach can be applied to the problem of electron transport in quantum dot, both in the linear response and non-equilibrium steady state regimes.

We illustrate this approach for the Anderson impurity model [3], which has not only played an important role in understanding the effects of magnetic impurities in metals (Kondo effect), but is also a basic model for describing the transport of electrons in nanoscale systems, and in particular quantum dot. The Hamiltonian for this model is

$$H = \sum_{\sigma} \epsilon_{d,\sigma} d_{\sigma}^{\dagger} d_{\sigma} + U n_{d,\uparrow} n_{d,\downarrow} + \sum_{k,\sigma} (V d_{\sigma}^{\dagger} c_{k,\sigma} + V^{*} c_{k,\sigma}^{\dagger} d_{\sigma}) + \sum_{k,\sigma} \epsilon_{k,\sigma} c_{k,\sigma}^{\dagger} c_{k,\sigma}. \quad (2.1)$$

The three basic parameters that specify the model are the energy level of the impurity state  $\epsilon_d$ , the hybridization width parameter  $\Delta = \pi |V|^2 \rho_c$  for a constant conduction band density of states  $\rho_c$ , and the interaction at the impurity site  $U$ . These will be replaced by the corresponding renormalized quantities,  $\tilde{\epsilon}_d$ ,  $\tilde{\Delta}$ , and  $\tilde{U}$ , defined by the equations,

$$\tilde{\epsilon}_d = z(\epsilon_d + \Sigma(0)), \quad \tilde{\Delta} = z\Delta, \quad \tilde{U} = z^2 \Gamma_{\sigma,-\sigma}^{(4)}(0, 0, 0, 0), \quad (2.2)$$

where  $\Sigma(\omega)$  is the self-energy of the impurity retarded Green’s function  $G_{d,\sigma}(\omega) = (\omega - \epsilon_d + i\Delta - \Sigma(\omega))^{-1}$ ,  $z = (1 - \Sigma'(0))^{-1}$  is the usual wavefunction

renormalization factor, and  $\Gamma_{\sigma,-\sigma}^{(4)}(\omega_1, \omega_2, \omega_3, \omega_4)$  is local full four vertex for the scattering of electrons with opposite spin. With this choice the Green's function  $G_{d,\sigma}(\omega)$  can be re-expressed in the form,  $G_{d,\sigma}(\omega) = z\tilde{G}_{d,\sigma}(\omega)$ , where  $z\tilde{G}_{d,\sigma}(\omega)$  is the quasiparticle Green's function given by

$$\tilde{G}_{d,\sigma}(\omega) = \frac{1}{\omega - \tilde{\epsilon}_d + i\tilde{\Delta} - \tilde{\Sigma}(\omega)}, \quad (2.3)$$

and the renormalized self-energy  $\tilde{\Sigma}(\omega) \sim \omega^2$  as  $\omega \rightarrow 0$ , assuming the Luttinger result that  $\text{Im}\Sigma(\omega) \sim \omega^2$ . The perturbation theory in powers of  $U$  can be reorganized into one in terms of the renormalized interaction  $\tilde{U}$ , with the free quasiparticle Green's function  $\tilde{G}_{d,\sigma}^0(\omega) = (\omega - \tilde{\epsilon}_d + i\tilde{\Delta})^{-1}$  as the propagator [4, 5]. Three counter terms have to be included to prevent any further renormalization of the parameters,  $\tilde{\epsilon}_d$ ,  $\tilde{\Delta}$ , and  $\tilde{U}$ , which have been taken to be fully renormalized. The counter terms can be determined order by order from the conditions,

$$\tilde{\Sigma}(0) = 0, \quad \tilde{\Sigma}'(0) = 0, \quad \tilde{\Gamma}_{\sigma,-\sigma}^{(4)}(0, 0, 0, 0) = \tilde{U}. \quad (2.4)$$

These are equivalent to the renormalization conditions used in field theory, but in this context they have nothing to do with the elimination of infinities, and are best regarded as overcounting conditions. This implies that the results of the model can now be specified entirely in terms of the three renormalized parameters,  $\tilde{\epsilon}_d$ ,  $\tilde{\Delta}$ , and  $\tilde{U}$ .

The advantage of the renormalized perturbation theory (RPT) is that the exact results in the low energy Fermi liquid regime can all be derived from the perturbation expansion to second order in  $\tilde{U}$  only. The Friedel sum rule which gives the occupation of the impurity site  $\langle n_{d,\sigma} \rangle$  takes the form,

$$\langle n_{d,\sigma} \rangle = \frac{1}{2} - \frac{1}{\pi} \tan^{-1} \left( \frac{\tilde{\epsilon}_d}{\tilde{\Delta}} \right), \quad (2.5)$$

and the impurity spin and charge susceptibilities at  $T = 0$ ,  $\chi_s$  and  $\chi_c$ , are given by

$$\chi_s = \frac{(g\mu_B)^2 \tilde{\rho}(0)}{2} (1 + \tilde{U} \tilde{\rho}(0)), \quad \chi_c = \frac{\tilde{\rho}(0)}{2} (1 - \tilde{U} \tilde{\rho}(0)). \quad (2.6)$$

where  $\tilde{\rho}(\omega)$  is the non-interacting quasiparticle density of states given by

$$\tilde{\rho}(\omega) = \frac{1}{\pi} \frac{\tilde{\Delta}}{(\omega - \tilde{\epsilon}_d)^2 + \tilde{\Delta}^2}. \quad (2.7)$$

The impurity contribution to the low temperature conductivity  $\sigma(T)$  for the symmetric model ( $\tilde{\epsilon}_d = 0$ ) is given by

$$\sigma_{\text{imp}}(T) = \sigma_0 \left\{ 1 + \frac{\pi^4}{3} \left( \frac{T}{\pi\tilde{\Delta}} \right)^2 \left( 1 + 2 \left( \frac{\tilde{U}}{\pi\tilde{\Delta}} \right)^2 \right) + \text{O}(T^4) \right\}. \quad (2.8)$$

In the nearly localized or Kondo regime,  $\tilde{\epsilon}_d \rightarrow 0$  and there is only one energy scale, the Kondo temperature  $T_K$ . In this regime,  $\chi_c \rightarrow 0$ , so from Eq. (2.6) we find  $\tilde{U} = \pi\tilde{\Delta}$ , so with  $T_K$  defined by  $\chi_s = (g\mu_B)^2/4T_K$ ,  $\tilde{U} = \pi\tilde{\Delta} = 4T_K$ .

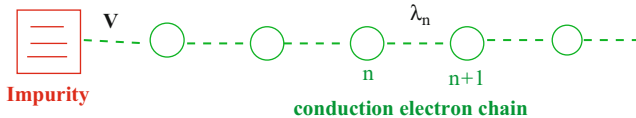
As no approximations have been made in setting up the renormalized perturbation theory, in principle results can be obtained appropriate to any energy scale if all the relevant diagrams can be taken into account. However, for calculations on higher energy scales we have to take account of the undressing or de-renormalization of the quasiparticles, which will involve higher order diagrams and terms to all orders in  $\tilde{U}$ , to recover the bare interaction  $U$  relevant on the high energy scale. The physical behavior on the low energy scale, however, is the one that is of most interest in strongly correlated electron systems. On this scale where the quasiparticles remain largely intact, the repeated scattering of quasiparticles can be readily taken into account in the renormalized perturbation theory. Explicit calculations of the local dynamic spin susceptibility using the RPT, taking these repeated scatterings into account, have been shown to give a very good account of the behaviour of this quantity on energy scales up to several times the Kondo temperature [6].

The disadvantage of the renormalized perturbation approach is that the renormalized parameters of the theory are unknown. As the number of relevant parameters can be small, one possibility is that they can be calculated by direct appeal to experiment, as in QED or Fermi liquid theory, and in the Kondo regime there is only a single parameter  $T_K$  to be determined. However, if the bare parameters are known, the renormalized parameters may be calculated by other means. In the next section we show, in the case of the Anderson model, how they can be calculated using the Wilson numerical renormalization group (NRG) approach.

## 2.2 Calculation of renormalized parameters

The Anderson model has to be cast into a slightly different form to carry out the NRG calculations [7]. The conduction band is discretized and converted to take the form of a tight-binding chain with the impurity coupled by the hybridization parameter  $V$  to the end site of the chain, as indicated in Fig. 2.1. The Hamiltonian then takes the form,

$$H = \sum_{\sigma} \epsilon_{d,\sigma} d_{\sigma}^{\dagger} d_{\sigma} + U n_{d,\uparrow} n_{d,\downarrow} + V \sum_{\sigma} (d_{\sigma}^{\dagger} c_{0,\sigma} + c_{0,\sigma}^{\dagger} d_{\sigma}) + \sum_{i,\sigma} \lambda_i (c_{i+1,\sigma}^{\dagger} c_{i,\sigma} + h.c.), \quad (2.9)$$



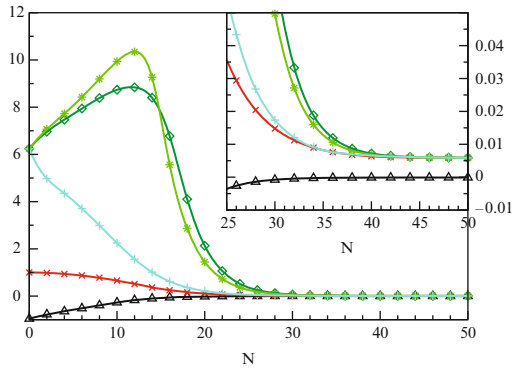
**Fig. 2.1.** Linear chain form of the Anderson model used for the NRG iteration scheme.

when the Fermi level is at the centre of the conduction band, where  $\lambda_i$  are the nearest neighbor hopping matrix elements along the conduction band chain. Iterative calculations are then carried out, starting at the impurity site and adding a conduction electron site with each iteration. Truncation has to be carried out when the number of states involved becomes too large to carry out the diagonalization. Only the lowest energy states are retained, so that as the states are retained, so that as the interaction progresses, the many-body energy lower energy scales. Further details on the setting up the NRG in this form can be found in the original papers [7] and a recent review article [8].

For this discretized model, the Green's function for the impurity site for  $U = 0$  takes the form,

$$G_{d,\sigma}^0(\omega) = \frac{1}{\omega - \epsilon_d - V^2 g_0(\omega)}, \quad (2.10)$$

where  $g_0(\omega)$  is the Green's function for the first site ( $i = 0$ ) on the conduction band chain in the absence of the impurity. The single particle excitations correspond to the poles of this Green's function. The quasiparticle Green's function for the interacting system, given in Eq. (2.3), takes a similar form at low frequencies when we can ignore the renormalized self-energy term  $\tilde{\Sigma}(\omega)$ . Then the lowest energy single particle and single hole excitations of the interacting system for the  $N$ th iteration,  $E_{N,p}$  and  $E_{N,h}$ , when  $N$  is large correspond to the very low energy regime, should correspond to the poles of (2.10) with  $\epsilon_d \rightarrow \tilde{\epsilon}_d$  and  $V \rightarrow \tilde{V}$  (equivalent to  $\Delta \rightarrow \tilde{\Delta}$ ). If this is the case then in the large  $N$  regime, the values deduced for  $\tilde{\epsilon}_d$  and  $\tilde{\Delta}$  should be independent of  $N$ . That this is the case is illustrated in Fig. 2.2, where the values deduced for  $\tilde{\epsilon}_d$  and  $\tilde{\Delta}$  as a function of  $N$  are given for a model in the Kondo regime, with  $\pi\Delta = 0.05$ ,  $\epsilon_d = -0.2$  and  $U = 0.3$ . The values for the two renormalized parameters  $\tilde{\epsilon}_d$  and  $\tilde{\Delta}$  can be deduced in this way (for further details see [9]).



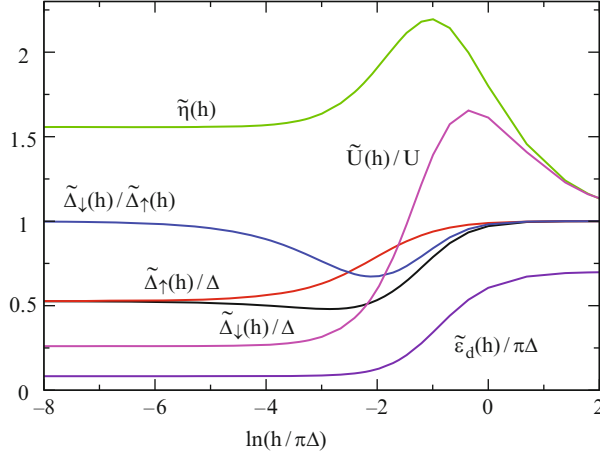
**Fig. 2.2.** Renormalized parameters:  $\tilde{\epsilon}_d$  (triangles),  $\pi\tilde{\Delta}$  (crosses),  $\tilde{U}_{pp}$  (stars),  $\tilde{U}_{hh}$  (squares), and  $\tilde{U}_{ph}$  (plus signs) as a function of the chain length  $N$  in units of  $\pi\Delta$  for the parameters  $\pi\Delta = 0.05$ ,  $\epsilon_d = -0.2$  and  $U = 0.3$ .

When considering excitations from the interacting ground state, which is taken to be the vacuum state, the interaction term does not come into play until we create two or more single particle excitations. If we create the lowest two-particle excitation, corresponding to an energy  $E_{N,pp}$  then, if there is an interaction between the quasiparticles, this will differ from the energy corresponding to the two non-interacting particles. The difference  $E_{N,pp} - 2E_{N,p}$  will be proportional to the interaction  $\tilde{U}_{pp}$  between the quasiparticles. We can similarly define an interaction  $\tilde{U}_{hh}$  between two holes, or  $-\tilde{U}_{ph}$ , between a particle and hole. If these excitations correspond to a renormalized Anderson model, then we should find for large  $N$  that  $\tilde{U}_{pp} = \tilde{U}_{hh} = \tilde{U}_{ph}$ , and we can identify the common value with  $\tilde{U}$ . The values deduced for  $\tilde{U}_{pp}$ ,  $\tilde{U}_{hh}$  and  $\tilde{U}_{ph}$  as a function of  $N$  are also given in Fig. 2.2. It can be seen that for large  $N$  they do indeed converge to a common value  $\tilde{U}$ . What is more, because we are in the Kondo regime, we see from the inset that they correspond to a single energy scale,  $\tilde{\epsilon}_d \sim 0$ ,  $\tilde{U} = \pi\tilde{\Delta}$ , as deduced from the RPT. We are, therefore, justified in identifying the  $\tilde{U}$  deduced from the NRG with the one defined in Eq. (2.2).

From the NRG calculation we have been able to calculate all three renormalized parameters required for the renormalized perturbation theory (RPT). The obvious question at this stage, is why do we need the RPT if we can calculate the physical quantities of interest directly using the NRG? There are two answers to this question. First of all it can be a very useful aid to the NRG. For instance, the calculation of the zero temperature susceptibility from the NRG is quite complicated, involving a subtraction from the total susceptibility of the result for the isolated conduction chain. Instead of this we can calculate the renormalized parameters,  $\tilde{\epsilon}_d$ ,  $\tilde{\Delta}$ , and  $\tilde{U}$ , and substitute into Eq. (2.6) which gives results accurate to four significant places when compared with the exact values calculated via the Bethe ansatz [9]. The renormalized parameters calculated for the physical ranges of  $U$  and  $\epsilon_d$  provide a global view of the low energy physics of the model (see Refs. [9, 10]). We can also generalize the approach and calculate the parameters as a function of an external magnetic field  $H$  and follow how the quasiparticles are de-renormalized from strongly renormalized values in the Kondo regime for weak fields, to bare values in extremely large fields when the low energy spin excitations responsible for the Kondo effect are suppressed [11, 12]. An example is shown in Fig. 2.3 where the parameters  $\epsilon_d(h)$  and  $\tilde{\eta}(h)$  are defined by  $0.5(\tilde{\epsilon}_{d,\downarrow}(h) + \tilde{\epsilon}_{d,\uparrow}(h))$  and  $0.5(\tilde{\epsilon}_{d,\downarrow}(h) - \tilde{\epsilon}_{d,\uparrow}(h))/h$ , respectively. For the asymmetric model shown  $\tilde{\Delta}_\sigma(h)$ , depend on the spin component  $\sigma$  in intermediate field regimes.

An advantage of the RPT is that the  $T^2$  coefficient in the impurity contribution to the conductivity can be calculated essentially exactly from Eq. (2.8). Due to problems of broadening, in obtaining a continuous spectrum from the discrete NRG results, this temperature dependence is difficult to calculate accurately from the NRG.

A major problem arises in extending the NRG method to non-equilibrium situations which occur, for instance, in calculating the current through a



**Fig. 2.3.** Renormalized parameters as a function magnetic field  $h = g\mu_B H/2$  for bare parameters  $\pi\Delta = 0.1$ ,  $U/\pi\Delta = 3.0$  and  $\epsilon_d/\pi\Delta = -0.3$  taken from Ref. [12].

quantum dot when a finite bias voltage is applied. Some progress with this problem has been made [13–15], but it is computationally very difficult, and there is clearly room for alternative methods. In the next section we see how the RPT can be applied to this class of problems.

### 2.3 Electron transport through quantum dot

The Anderson impurity model has almost universally been used to describe the electron transport through a quantum dot, coupled by leads to two electron reservoirs, when a bias voltage  $V_B$  is applied between the reservoirs to induce a current flow through the dot. The model is appropriate to the Coulomb blockade regime when the spacing between the energy levels on the dot are large, and the coupling through the leads is relatively weak. The difference with the model as described in Eq. (2.1), where the impurity plays the role of the dot, is that there is a coupling or hybridization with two electron reservoirs. This means that the hybridization term in Eq. (2.1) is replaced by two such terms, with the  $V_L$  the coupling via the left lead to the  $L$ -reservoir of electrons, and  $V_R$  to the right lead and the  $R$ -reservoir, where  $\sum_{k,\sigma} \epsilon_{k,\sigma} c_{i,k,\sigma}^\dagger c_{i,k,\sigma}$  for  $i = L, R$  describes the two electron reservoirs. Using this model and the Keldysh generalization of perturbation theory for non-equilibrium but steady state conditions, Meir and Wingreen [16] derived the formula for the current  $I$  passing through the quantum dot,

$$I = \frac{2e\Delta_L\Delta_R}{\pi\hbar(\Delta_L + \Delta_R)} \sum_{\sigma} \int_{-\infty}^{+\infty} (f_L(\omega) - f_R(\omega)) [-\text{Im } G_{d,\sigma}^r(\omega, V_B)] d\omega, \quad (2.11)$$

where  $G_{d,\sigma}^r(\omega, V_B)$  is the retarded Green's function for the dot site calculated under steady state conditions, and  $f_L(\omega)$ ,  $f_R(\omega)$  are the Fermi distribution functions for the electrons in the left and right reservoirs, respectively. The Green's function  $G_{d,\sigma}^r(\omega, V_B)$  is the same form as defined earlier after Eq. (2.2), with  $\Delta$  replaced by  $\Delta_L + \Delta_R$ , but the self-energy  $\Sigma_\sigma(\omega, V_B)$  in the presence of a finite bias voltage  $V_B$  has to be calculated under steady state conditions using the more general Keldysh perturbation theory [17]. The chemical potentials in the left and right channel,  $\mu_L$  and  $\mu_R$ , are such that  $\mu_L - \mu_R = eV_B$ .

For the calculation to first order in  $V_B$  at zero temperature, we need only the Green's function at  $\omega = 0$ , as the Fermi factors give a term in  $V_B$ . This is given by  $z$  multiplied by the quasiparticle Green's function given in Eq. (2.3) with  $\tilde{\Sigma}(0) = 0$ . Then

$$\frac{\partial I}{\partial V_B} = \frac{4e^2}{\pi\hbar} \frac{\tilde{\Delta}_L \tilde{\Delta}_R}{\tilde{\epsilon}_d^2 + (\tilde{\Delta}_L + \tilde{\Delta}_R)^2}, \quad (2.12)$$

which is entirely in terms of renormalized parameters. A similar quasiparticle approach to the zero-temperature conductance has been developed by Rejec and Ramšak [18]. The result can alternatively be expressed in terms of a phase shift  $\eta$ ,

$$\frac{\partial I}{\partial V_B} = \frac{4e^2}{\pi\hbar} \frac{\Delta_L \Delta_R}{(\Delta_L + \Delta_R)^2} \cos^2 \eta, \quad (2.13)$$

where  $\eta = \tan^{-1}(\tilde{\epsilon}_d/(\tilde{\Delta}_L + \tilde{\Delta}_R))$ .

This approach has been generalized to calculate the differential conductivity through more complicated multidot systems [19–21]. It can also be generalized to include an arbitrary magnetic field to give

$$\frac{\partial I}{\partial V_B} = \frac{2e^2}{\pi\hbar} \sum_{\sigma} \frac{\tilde{\Delta}_{\sigma,L}(h) \tilde{\Delta}_{\sigma,R}(h)}{(\tilde{\epsilon}_d(h) - \sigma h \tilde{\eta}(h))^2 + (\tilde{\Delta}_{\sigma,L}(h) + \tilde{\Delta}_{\sigma,R}(h))^2}. \quad (2.14)$$

Once the renormalized parameters have been calculated, these expressions can be evaluated by direct substitution into the formulae.

As an exact expression can be derived for the self-energy  $\tilde{\Sigma}(\omega)$  from the RPT to order  $T^2$  and  $\omega^2$ , the coefficient of the leading order  $T^2$  correction to the linear response can be calculated exactly. The result for the renormalized self-energy for the symmetric model ( $\epsilon_d = -U/2$ ) is

$$\tilde{\Sigma}(\omega, T) = -\frac{i\tilde{U}^2}{2\pi^2(\tilde{\Delta}_L + \tilde{\Delta}_R)^3} [\omega^2 + (\pi T)^2 + \dots], \quad (2.15)$$

which then leads to

$$\frac{\partial I}{\partial V_B} = \frac{4e^2}{\pi\hbar} \frac{\tilde{\Delta}_L \tilde{\Delta}_R}{(\tilde{\Delta}_L + \tilde{\Delta}_R)^2} \left[ 1 - \frac{1 + 2(R-1)^2}{3} \left( \frac{\pi T}{\tilde{\Delta}_L + \tilde{\Delta}_R} \right)^2 + \dots \right], \quad (2.16)$$



where  $R = 1 + \tilde{U}/\pi(\tilde{\Delta}_L + \tilde{\Delta}_R)$ . In the Kondo regime, the model is essentially symmetric as  $\tilde{\epsilon}_d \rightarrow 0$ ,  $\tilde{U} = \pi(\tilde{\Delta}_L + \tilde{\Delta}_R) = 4T_K$  and  $R = 2$ .

Techniques for calculating the local equilibrium Green's function using the NRG, for models like the Anderson model, have now become almost standard, and the results can be substituted directly into the Meir-Wingreen formula (2.11) to evaluate the linear response. Going beyond the linear response regime, to calculate the Green's function in non-equilibrium situations is a much more demanding problem. Progress has been made in extending the NRG technique to quantum dot models in non-equilibrium [13–15], and also in applying the Bethe ansatz approach [22]. Any definitive results obtained using these approaches would give useful benchmarks for testing approximation schemes which might be applicable to a wider class of models. The RPT approach can rather straightforwardly be extended to steady state non-equilibrium conditions using the renormalized version of the Keldysh perturbation theory [17]. The free propagators used in the expansion can be expressed in terms of the renormalized parameters,  $\tilde{\epsilon}_d$ ,  $\tilde{\Delta}_L$  and  $\tilde{\Delta}_R$  to calculate the renormalized self-energy  $\tilde{\Sigma}(\omega)$ , to evaluate the retarded quasi-particle Green's function as given in Eq. (2.3). A systematic expansion can be developed in powers of  $\tilde{U}$ . To zero order in  $\tilde{U}$ , and symmetric couplings,  $\tilde{\Delta}_L = \tilde{\Delta}_R = \tilde{\Delta}/2$

$$\frac{\partial I}{\partial V_B} = \frac{e^2}{2\pi\hbar} \left[ \frac{\tilde{\Delta}^2}{(\tilde{\epsilon}_d - eV_B/2)^2 + \tilde{\Delta}^2} + \frac{\tilde{\Delta}^2}{(\tilde{\epsilon}_d + eV_B/2)^2 + \tilde{\Delta}^2} \right]. \quad (2.17)$$

In the Kondo regime with  $\tilde{\Delta} = 4T_K/\pi$ , this simplifies to

$$\frac{\partial I}{\partial V_B} = \frac{e^2}{\pi\hbar} \frac{T_K^2}{(e\pi V_B/8)^2 + T_K^2}, \quad (2.18)$$

which, as a function of  $eV_B$ , corresponds to a resonance of width of the order  $T_K$ .

When carried out to second order in  $\tilde{U}$ , the leading order correction to the renormalized self-energy to order  $V_B^2$ , assuming symmetric couplings, is  $-3i\tilde{U}^2(eV_B)^2/8\pi^2\tilde{\Delta}^3$ . When this term is taken into account, the leading corrections to the  $T = 0$  linear differential conductance are given by

$$\frac{\partial I}{\partial V_B} = \frac{e^2}{\pi\hbar} \left[ 1 - \frac{1 + 2(R-1)^2}{3} \left( \frac{\pi T}{\tilde{\Delta}} \right)^2 + \frac{1 + 5(R-1)^2}{4} \left( \frac{eV_B}{\tilde{\Delta}} \right)^2 \dots \right], \quad (2.19)$$

This result is exact to order  $V_B^2$  as well as to order  $T^2$  as first shown by Oguri [23, 24]. The result is applicable in the Kondo regime, with  $\tilde{U} = \pi\tilde{\Delta} = 4T_K$ .

In theoretical calculations it is often useful to simplify matters by making the coupling to the two leads equal,  $\Delta_L = \Delta_R$ , and assume particle-hole

symmetry, so that one can take  $\mu_L = \mu + eV_B/2$  and  $\mu_R = \mu - eV_B/2$ . With this symmetry the charge on the dot will not change as the bias voltage is varied. Experimentally this situation is difficult to achieve, and the relative coupling to two leads can be an important factor. In the extreme case that one of the leads is only weakly coupled to the dot, so that  $\Delta_L \gg \Delta_R$ , then it should be reasonable to assume that the current into the right reservoir is probing the equilibrium situation of the dot. If this is the case, it should be sufficient to leading order in  $\Delta_L$  to use the equilibrium Green's function on the dot in evaluating the current using the Meir-Wingreen formula (2.11). This is the usual assumption in STM experiments where the probe of the microscope is weakly coupled to the atoms which are probed on the surface being examined. If this is not the case, then the effects of asymmetry in the coupling strengths needs to be considered carefully. One way of parameterizing the dependence of the left and right chemical potentials on the bias voltage  $V_B$  is  $\mu_L = \mu + \alpha_L eV_B$ ,  $\mu_R = \mu - \alpha_R eV_B$ , such that  $\alpha_L + \alpha_R = 1$ , but  $\alpha_L - \alpha_R$  is undetermined. In the absence of a bias voltage the values of the energy level on the dot,  $\epsilon_d$ ,  $\epsilon_d + U$  (measured relative to  $\mu$ ), will largely determine the charge on the dot. Applying a gate voltage to the dot allows these levels to be moved so that current through the dot can be measured in different parameter regimes for the charge on the dot. The factor  $\alpha_L - \alpha_R$  introduces a bias voltage dependent shift in  $\epsilon_d$ , so that the charge on the dot may change as the bias voltage is varied. If the charge on the dot is known as a function of the bias voltage then this information can be used to determine  $\alpha_L$  and  $\alpha_R$  individually. This means that for a complete calculation of the current through the dot one needs also to be able to calculate the charge on the dot in steady state conditions with an applied bias voltage. The zero order result, Eq. (2.17), generalizes to

$$\frac{\partial I}{\partial V_B} = \frac{4e^2}{\pi\hbar} \left[ \frac{\alpha_L \tilde{\Delta}_L \tilde{\Delta}_R}{(\tilde{\epsilon}_d - \alpha_L eV_B)^2 + \tilde{\Delta}^2} + \frac{\alpha_R \tilde{\Delta}_L \tilde{\Delta}_R}{(\tilde{\epsilon}_d + \alpha_R eV_B)^2 + \tilde{\Delta}^2} \right], \quad (2.20)$$

with asymmetric couplings, where  $\tilde{\Delta} = \tilde{\Delta}_L + \tilde{\Delta}_R$ . The corresponding result for the charge on the dot is

$$\langle n_{\text{dot}} \rangle = 1 + \frac{2\tilde{\Delta}_L}{\tilde{\Delta}} \tan^{-1} \left( \frac{\tilde{\epsilon}_d - \alpha_L eV_B}{\tilde{\Delta}} \right) + \frac{2\tilde{\Delta}_R}{\tilde{\Delta}} \tan^{-1} \left( \frac{\tilde{\epsilon}_d + \alpha_R eV_B}{\tilde{\Delta}} \right). \quad (2.21)$$

It can be shown, however, that in the calculation of the  $V_B^2$  term in the differential conductivity that if one assumes  $\Delta_L \neq \Delta_R$ , the result of the evaluation of the integral in Eq. (2.11) to this order is independent of  $\alpha_L - \alpha_R$ , so Eq. (2.19) can be generalized to the case of unequal couplings by multiplying the result in (2.19) by a factor  $4\Delta_L\Delta_R/(\Delta_L + \Delta_R)^2$ .

There have been some very careful experiments on quantum dot in the Kondo regime, which have been used to estimate some of these leading correction terms [25] to the differential conductance, plus an estimate of further

correction term proportional to  $V_B^2 T^2$ . The results are consistent both with the  $V_B^2$  and  $T^2$  power law, and also general agreement with the magnitude of the coefficient as given in Eq. (2.19). An analysis of these results, including the  $V_B^2 T^2$  term, has been made by Rincón et al. [26] using the non-equilibrium RPT to second order for the Anderson model. They find for a value of  $\tilde{U}/\pi\tilde{\Delta} = 0.365$ , which corresponds to a regime in which charge fluctuations play a role, that they get excellent agreement with the experimental results, including the coefficient of the term in  $V_B^2 T^2$ .

Experiments have also been made of the transmission through a quantum dot in the Kondo regime in the presence of a magnetic field [27–29]. They have been used to make estimate of the splitting of a Kondo resonance by a magnetic field, with results that are claimed to be disagreement with theory. However, these experiments are performed by measuring the transmission by varying the bias voltage, and there are no definite predictions of any precise theory so far of the current through a dot under these non-equilibrium conditions. Using the RPT it is possible to extend the calculations of the leading order corrections to the differential conductance as given in Eq. (2.19) to situations with arbitrary strength magnetic field, via using the field dependent renormalized parameters, as in Eq. (2.14). As the magnetic field strength is increased, there is a critical value at which the  $V_B^2$  term in the expression for the total differential conductivity changes sign. This is the signal for two peaks to begin to emerge in the differential conductivity as  $V_B$  is varied. This critical field can be calculated exactly, as the coefficient of the  $V_B^2$  is given exactly by the RPT and the renormalized parameters are valid for arbitrary magnetic field. The details of this calculation are rather more complicated, so we will not reproduce the result here but refer to the paper of Hewson et al. [30].

The  $T^2$  coefficient in Eq. (2.19) also becomes field dependent in the presence of a magnetic field. Again this can be calculated exactly using field dependent renormalised parameters [11, 12]. As the field strength increases this coefficient also changes sign for a value of order  $\hbar \sim T_K$ . The values of  $T_K$  should be small enough in some quantum dot for this change of sign to be seen experimentally.

A further exact result for quantum dot has been established using RPT by Fujii [31]. He has derived a result for the shot noise  $S_h$  to leading order in  $V_B$  for the model with symmetric couplings,

$$S_h = \frac{2e^3|V_B|}{\pi\hbar} \left[ \frac{1}{12} \left( \frac{eV_B}{\tilde{\Delta}} \right)^2 + \frac{3(R-1)^2}{4} \left( \frac{eV_B}{\tilde{\Delta}} \right)^2 \dots \right], \quad (2.22)$$

which corresponds to the result derived for the s-d model [32] in the Kondo regime when  $R = 2$ .

## 2.4 Discussion

The renormalized perturbation theory is a way of carrying out a perturbation expansion in terms of fully dressed quasiparticles. No approximations are made in setting up the expansion, so in principle it can be used for calculations in any energy or parameter regime. The method is most useful, however, in the low energy regime where the physics is dominated by quasiparticle scattering, and asymptotically exact results can be obtained from either low order perturbation theory alone, or from a subclass of diagrams involving repeated quasiparticle scattering. In a strongly correlated system, it is the low energy regime where most of the interesting physics takes place. The renormalized parameters have to be determined, and they can be calculated very accurately for impurity models using the NRG. The approach is a very useful adjunct to the NRG. The approach is not dependent on the NRG, however, and it should be possible to calculate the renormalized parameters in other ways, and some of these alternatives are being examined.

In quantum dot the physics of strongly correlated systems can be explored in equilibrium and steady state conditions. The fact that many of the important parameters can be varied in controlled ways, by changing applied gate voltages, or the number or geometry of the dots, means that theoretical predictions can be tested over physically distinct parameter regimes. The RPT approach has proved useful in analysing the conduction through more complicated arrangements of quantum dot [19–21]. In applying the method to non-equilibrium steady state conditions, it is encouraging that a number of exact asymptotic results can be established from calculations carried out to second order only. There is certainly scope for extending the calculations to higher energy scales, and higher bias voltage, by taking account of higher order scattering processes.

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